32

New resource-sparing grid methods for solving the problems of mathematical physics

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Abstract

The solution of new classes of application problems in the fields of continuum mechanics, including the problems of three-dimensional aerodynamics and hydrodynamics, space physics, and environmental science often require considerable computer resources which are often too great even for the leading and best equipped research centers. We believe this problem can be solved by employing up-to-date methods based on irregular adapting grids. For the solution of two-dimensional elliptic problems an adaptive projection-grid method has been designed. The solution is sought as a piecewise-polynomial function. Overdetermined system collocation equations of the differential equation and special mixed conform conditions are used for defining of the coefficients of these polynomials. It is sought on a sequence of grids adapted to the singularities of the solution and to the domain geometry, see also Shokin, Sleptsov (1995) and Sleptsov, Shokin (1995).

Comprehensive grid generation method which enables the user to generate both adaptive and fixed grids in a unified manner on surfaces and in domains was developed. Namely the adaptive grid in the domain is formed as the projection of the uniform grid from a monitor surface. The method relies on a variational approach of generating uniform grids on hypersurfaces, see Liseikin (1991).

Keywords

Irregular adapting grids, two-dimensional elliptic problems, adaptive projection–grid method, piecewise-polynomial function, system collocation equations, mixed conform conditions

R. F. Boisvert (ed.), *Quality of Numerical Software*

1 AN ADAPTIVE PROJECTION-GRID METHOD FOR THE SOLUTION OF TWO-DIMENSIONAL ELLIPTIC PROBLEMS

1.1 Introduction

In the solution of elliptical problems with a small parameter of higher derivatives boundary and/or internal layers may arise. Adaptive methods are required. In the grid methods the grid must be significantly condensed in the vicinity of those layers in order to get a good solution without consuming too much computer time. Most methods of this kind (finite-difference or projection grid) are not when the cell deformations are great, see Aubin (1972), Ciarlet (1978), Strang, Fix (1973).

1.2 Approximation equations

Let us consider the boundary problem written in the Cartesian rectangular system of coordinates:

$$a_{11}v_{x_1x_1} + a_{12}v_{x_1x_2} + a_{22}v_{x_2x_2} + b_1v_{x_1} + b_2v_{x_2} + cv = f, \quad (x_1, x_2) \in \Omega, \tag{1}$$

$$\gamma(\mathbf{x})\frac{\partial v(\mathbf{x})}{\partial \mathbf{s}} + \delta(\mathbf{x})v(\mathbf{x}) = \lambda(\mathbf{x}), \quad \mathbf{x} = (x_1, x_2) \in \partial\Omega. \tag{2}$$

Here $a_{11} = a_{11}(x_1, x_2)$, $a_{12} = a_{12}(x_1, x_2)$, ...; $\mathbf{s}$ is the unit vector of the external normal. Let us assume that Equ. (1) is elliptical, the problem (1), (2) is uniquely solvable and its solution is a sufficiently smooth function.

In order to obtain an approximated solution of the problem (1), (2) let us introduce in the Ω domain triangulation $\Im = \{T_i\}_1^I$ where T_i are triangles among which there can be also curvilinear triangles if they are adjacent to the boundary of the domain $\partial\Omega$. The approximated solution is sought in the form of a piecewise quadratic function. For its representation in the triangle T_i and in order to obtain the respective system of equations we shall introduce local coordinates $(y_1^{(i)}, y_2^{(i)})$ which are obtained from the initial system of coordinates by means of tension, shear and turn. The approximate solution of the problem in the triangle T_i is sought in the form of a quadratic polynomial.

$$\tilde{u}(y_1, y_2) = p_{1i} + p_{2i}y_1 + p_{3i}y_2 + p_{4i}y_1^2 + p_{5i}y_1y_2 + p_{6i}y_2^2. \tag{3}$$

On each boundary ∂T_{ij} between the triangles T_i and T_j we shall specify the conditions of coincidence

$$\frac{\partial v_i}{\partial \mathbf{s}_i} + \eta_i v_i = \frac{\partial v_j}{\partial \mathbf{s}_i} + \eta_i v_j, \quad \frac{\partial v_i}{\partial \mathbf{s}_j} + \eta_j v_i = \frac{\partial v_j}{\partial \mathbf{s}_j} + \eta_j v_j, \tag{4}$$

where $\mathbf{s}_i, \mathbf{s}_j$, are unit vectors of external normals to the triangles T_i and T_j, v_i and v_j are the functions specified in the triangles and respectively. Parameter η_i is the empirical function of p_i - the perimeter of the triangle T_i and d_i of the half of its greatest side, it has a form

of $\eta_i = \min(\zeta_0/p_i, \zeta_1, \zeta_2 p_i)/d_i$, where constants $\zeta_0, \zeta_1, \zeta_2$ were selected experimentally so as to diminish the number of iterations and increase the accuracy of calculations. After a great number of experiments we have taken the values $\zeta_0 = 1, \zeta_1 = 4, \zeta_2 = 100$.

On refining the solution in triangle T_i the coefficients of the polynomial $\bar{u}$ are obtained from the equations of the collocation of the Equ. (1) at m points inside the closed triangle T_i and at the n points of the first coincidence conditions (4) or boundary conditions (2) (if the triangle is adjacent to the domain boundary). The m equations of collocation of the Equ. (1) and the $3n$ equations of collocation of the first coincidence condition (4) (up to n equations on the each side of the triangle T_i) can be written in the following form:

$$\sum_{k=1}^{6} B_{kji} p_{ki} = F_j, \quad j = 1, \ldots, m + 3n. \tag{5}$$

Since $m > 1, n > 1$ this system is overdetermined. Under its solution we shall understand, as usual, vector $\mathbf{p}_{.,i}$ minimizing the functional

$$\Phi(\mathbf{p}_{.,i}) = \sum_{j=1}^{m+3n} \omega_j \sum_{k=1}^{6} (B_{kji} p_{ki} - F_j)^2.$$

Coefficients ω_j were selected experimentally. From the condition of the minimum of this functional we obtain a system of 6 linear algebraic equations

$$\sum_{k=1}^{6} \sum_{j=1}^{m+3n} \omega_j B_{jkk} B_{jli} p_{kj} = \sum_{j=1}^{m+3n} \omega_j B_{lji} F_j, \quad l = 1, \ldots, 6.$$

Therefore, we have a system of $6I$ equations with $6I$ unknowns where I is the number of triangles in the grid.

1.3 Topography of the grid and iterative process

We consider the grid as a set of planted trees. In this case the grid topography is described as a graph consisting of a certain set of planted trees Gardner (1988) (the similar method was employed in Ref. Atlas, Stephenson (1991), Oden, Demkowicz (1991) for the description of irregular grids). At the first stage a certain set of N root triangle meshes $\{T_i\}_{i=1}^{I}$. In the course of more precise definition of the solution described later all or some meshes are divided and an approximated solution is calculated on the new grid. Then some of the cells are divided again and so on until the required accuracy is achieved or the allocated memory is exhausted.

In order to solve the resulting system of linear algebraic equations the alternating Schwartz method is employed, see, for instance, Lebedev, Agoshkov (1983), Nepomnyatshikh (1986), Smelov (1982). In this method the initial approximation is specified, the domain is subdivided into subdomains and the solution is corrected during transition from one subdomain to another. In our case separate cells of the grid $\Im_I$ were subdomains. The by-pass of the grid in the first case was carried out successively - tree by tree. This method employs also the iteration convergence accelerating based on the method of

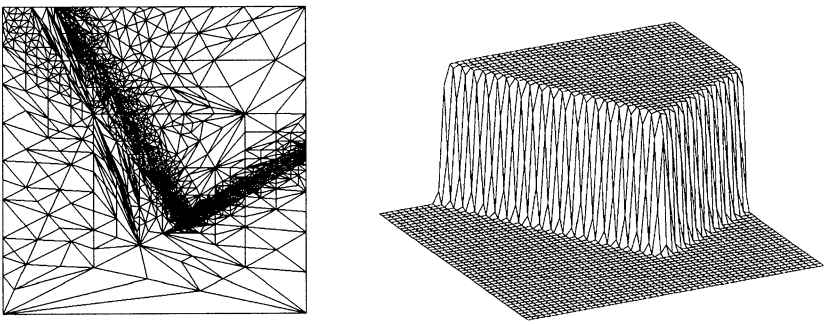

Figure 1 The mesh (a, left) and graph (b, right) of the solution of the example 1.

error projection onto the subspace of residuals i.e. EPSR-accelerating method (Sleptsov, 1991a, Sleptsov 1991b).

The calculations are carried out on the succession of grids. First a rough grid is specified. An approximated solution is obtained on this grid. After this the *estimator* is calculated $E(x_1, x_2) = E_i = const$ for $\mathbf{x} = (x_1, x_2) \in T_i$ where E_i is the local (defined in the triangle T_i) norm of the error estimate. The calculation of the estimator will be described in the next paragraph. Then the meshes for which the estimator value is high are further refined and the solution is calculated on the new grid $\Im_{I'}$. In this case the approximated solution obtained on the previous grid $\Im_I$ is used as the initial approximation.

1.4 Numerical experiments

These experiments were carried out with two model problems in which internal as well as boundary layers appearing in fields with a complicated form were considered.

Example 1. A model problem of diffusion-convection type

$$\epsilon \Delta u + (x_1 - a_1)u_{x_1} + (x_2 - a_2)u_{x_2} = 0. \tag{6}$$

This equation has the following family of exact solutions. Let φ be an angle and $\mu = \cos\varphi$, $\nu = \sin\varphi$, $p = -(\mu a_1 + \nu a_2)$, $q = \nu a_1 - \mu a_2$. Denote $y_1 = \mu x_1 + \nu x_2 + p$, $y_2 = -\nu x_1 + \mu x_2 + q$, $G(y) = 0.5 + \frac{1}{\sqrt{\pi}} \int_0^{y/\sqrt{\epsilon}} e^{-t^2} dt$.

Then, as it is easy to check, function $u(x_1, x_2) = G(y_1)G(y_2)$ will be the solution of equation (6). The solution of equation (6) was discovered in a unit square $\Omega = [0,1] \times [0,1]$ with boundary conditions $u(x_1, x_2)|_{\partial\Omega} = G(y_1)G(y_2)$. Under low values of the parameter ϵ function $u(x_1, x_2)$ will have internal layers. Under $\epsilon = 10^{-4}$, $\varphi = \pi/6$, $a_1 = 0.6$, $a_2 = 0.3$ the diagram of this function is shown in Figure 1. It actually coincides (with an accuracy to 1% in uniform norm) with the diagram of approximate piecewise-quadratic solution obtained on the grid shown in the same figure on the left. Figure 2 shows the dependence of the uniform and mean square norms of errors from the number of cells of grid I. The numbers on the upper curve in Figure 2 are the number of iterations (for certain points)

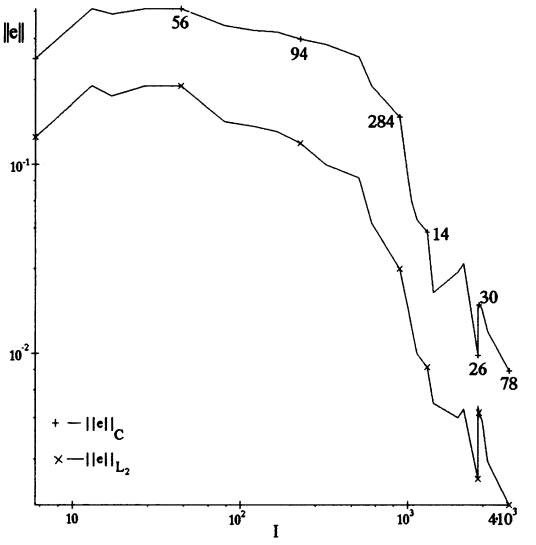

Figure 2 The dependence of the norms of the errors from numbers of cells.

which it is necessary to make for convergence. On such grids the error norms of the approximate solution considerably exceed the respective norms on adaptive grids.

Example 2. The solution of Helmholtz equation in a field of complicated polygonal shape

$$\epsilon\Delta u - u = \frac{10}{3}(x_1^2 + x_2^2)^2 - \frac{17}{6}(x_1^2 + x_2^2) + \frac{7}{10}, \quad (x_1, x_2) \in \Omega$$

$$u(x)\Big|_{\Gamma_1} = 0, \quad \frac{\partial u}{\partial n}\Big|_{\Gamma_2} = 0, \quad \frac{\partial u}{\partial n} + u\Big|_{\Gamma_3} = 0,$$

where area Ω and its boundaries Γ_i, $i = 1, 2, 3$, are shown in Figure 3. External angles of the star are uniformly distributed along the circle of radius (0., 1.) $R = 1$ and its first vertex has coordinates (0., 1.), the internal angles are on the circle with radius $r = 0.5$.

2 A NEW BASIC METHOD FOR COMPREHENSIVE GRID GENERATION

2.1 Introduction

Modern computational technologies for the numerical solution of field problems require for their successive application the development of Comprehensive Grid Generation Codes (CGGC) which will enable the users to generate grids with necessary properties in a unified

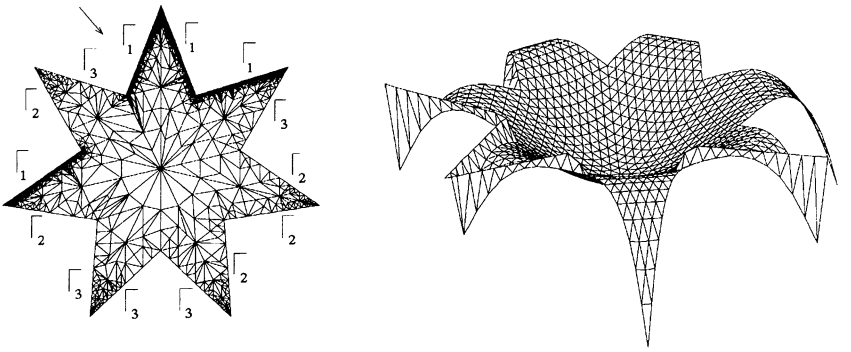

Figure 3 The mesh (a, left) and graph (b, right) of the solution of the example 2.

manner for a wide class of domains using state-of-the-art techniques. The efficiency of such CGGC is essentially dependent on a reliable basic method which provides an uniform environment for the construction of grids.

Present codes chiefly rely on the elliptic method, based on Poisson's equations with control functions providing adaptation. Other methods (algebraic, hyperbolic etc.) play an subsidiary role, namely they are applied as an initial guess for the elliptic solver or are used for the generation of grids in simple regions or for simple problems. However this basic method has at least two serious drawbacks.

- Control functions cannot provide efficient adaptation simultaneously in several intersecting directions.
- The cells of adaptive grids, obtained by the method can be overturned or degenerated even in domains with simple geometry, let alone in complex ones.

These drawbacks are being overcome in our Institute by developing a new basic method. The method relies on a variational approach of generating uniform grids on hypersurfaces (Liseikin, 1991). Using this approach one can generate both adaptive or fixed grids in a unified mode in domains as well as on their boundaries. Namely the adaptive grid in the domain is formed as a projection of the uniform grid from a monitor surface. The monitor surface is defined as a surface of some vector (weighting) function over the domain.

The vector function is determined by the physical solution, combination of its components, derivatives, or other variable quantities that must suitably monitor the solution behavior. The monitor surface is formed by values of the vector function $\mathbf{u}(x)$. The uniform grid on S is transformed into an adaptive grid in X by the operation of projecting. The uniform grid in X can be obtained by this approach when the monitor surface coincides with X. So the monitor surfaces can play the same role as a control functions in elliptic methods. But in comparison with the elliptic methods they can be determined more straightforwardly to provide efficient adaptation simultaneously in several intersecting narrow zones.

2.2 Formulation of the basic method

The method of generating uniform grids on hyper-surfaces relies on the minimization of a functional of grid smoothness (Liseikin, 1991, 1996a). We shall consider arbitrary n-dimensional hyper-surfaces lying in the $n+k$ dimensional space, though for the practical applications mostly important be $n = 2$ when generating adaptive grids on the boundaries and $n = 3$ for generating adaptive grids in domains.

So let S^{rn} be an n-dimensional surface in R^{n+k} with a local coordinate system $(s^1, \ldots, s^n) = s \in R^n$, defined by the non degenerate transform

$$r(s) : S^n \to S^{rn}, \quad r = (r^1, r^2, \ldots, r^{n+k}).$$

The numerical grid onto S^{rn} is defined by mapping the nodes of an uniform grid in some reference domain Q^n with the transform

$$r(s(q)) : Q^n \to S^{rn}, \quad (q^1, q^2, \ldots, q^n) = q \in Q^n,$$

which is the composition of $r(s)$ and some non degenerate mapping $s(q) : Q^n \to S^n$. The mapping $r(s(q))$ defines on the surface a new coordinate system $(q^1, q^2, \ldots, q^n) = q$ which generates the local metric tensor $\mathbf{G}^{rq} = \{\mathbf{g}_{ij}^{rq}\}$ $i, j = 1, 2, \ldots, n$, whose elements are products of the tangent vectors $\mathbf{r}_i = \partial \mathbf{r}/\partial q^i$, that is

$$\mathbf{g}_{ij}^{rq} = \mathbf{r}_i \mathbf{r}_j = \sum_{m=1}^{n+k} \frac{\partial \mathbf{r}^m}{\partial q^i} \frac{\partial \mathbf{r}^m}{\partial q^j} \tag{7}$$

and local contravariant metric tensor $\mathbf{G}_{qr} = \{\mathbf{g}_{qr}^{ij}\}$. These tensors satisfy the evident relation $\mathbf{G}^{rq}\mathbf{G}_{qr} = \mathbf{I}$.

The functional of grid smoothness on the surface S^{rn} is defined in the following form

$$F_s = \int_{S^{rn}} \mathrm{tr}(\mathbf{G}_{qr}) dS^{rn} = \int_{S^{rn}} \Big(\sum_{i=1}^{n} \mathbf{g}_{qr}^{ii}\Big) dS^{rn}.$$

In the particular case when the surface S^{rn} is a domain X (that is when adaptation is not required) the functional has the form:

$$F_s = \int_X \Big(\sum_{i=1}^{n} \mathbf{g}^{ii}\Big) dx,$$

where

$$\mathbf{g}^{ij} = \sum_{k=1}^{n} \frac{\partial q^k}{\partial x^i} \frac{\partial q^k}{\partial x^j}$$

and consequently it is the well known functional of smoothness suggested by Brackbill and Saltzman in 1982 for smoothing adaptive grids.

2.3 Geometrical interpretation

The smoothness functional can also be described in equivalent form (Liseikin, 1993):

$$F_s = \int_{S^{rn}} \left(\frac{I_{n-1}}{I_n}\right) dS^{rn},$$

where I_k, $k = n-1, n$ - denotes the kth invariant of all orthogonal transformations of the tensor S^{rq}. As $I_n^{1/2}$ is associated with the volume of an n-dimensional cell, and $I_{n-1}^{1/2}$ with the space of all its faces, it is evident that

$$\frac{I_{n-1}}{I_n} = c \sum_i^n \frac{1}{(l_i)^2},$$

where l_i is the distance between the coordinate surfaces in q_i-direction. Therefore the functional is an integral measure of grid clustering in all directions and consequently the problem of its minimization can be treated as a problem of finding a uniformly clustered grid or a uniform grid on the surface which turns out to be the adaptive grid after its projecting on the physical domain or its boundary.

2.4 Relation to harmonic functions

In terms of the theory of differential geometry the smoothness functional can be interpreted as a total energy associated with the mapping $q(s) : S^n \to Q^n$, which is inverse to $s(q) : Q^n \to S^n$ (Liseikin, 1993, 1996b). The function that delivers the minimum to the functional of energy is called harmonic. It follows from the theory that if the logic domain Q^n is convex and diffeomorphic to S^n than the harmonic function will presumably be one-to-one mapping. So by this method we can construct non-degenerate grids on simply connected domains or surfaces regardless the shape of their boundaries and therefore to eliminate the second drawback of the elliptic method.

2.5 Relation to the Tensor Laplace Equations

The function $q(s)$ giving the minimum to the functional of smoothness satisfy the system of Euler-Lagrange Equations:

$$L(q^i) = \sum_{j,k=1}^n \frac{\partial}{\partial s^j}\left(g_{qr}^{jk} \frac{\partial q^i}{\partial s^k}\right) = 0.$$

If a domain $X \subset R^n$ is considered as S^{rn}, then the system is equal to the system of the Laplace equations:

$$\Delta q^i = \sum_{j=1}^n \frac{\partial}{\partial x^j}\left(\frac{\partial q^i}{\partial x^j}\right) = 0, \quad i = 1, \ldots, n.$$

In our case it appears as well that the system of the Euler-Lagrange equations is equivalent to the system of Tensor Laplace equations. Namely (Liseikin, 1993, 1996a):

$$L(q^i) = \mathbf{g}\mathrm{div}(\mathbf{S}^{rs}(q^i)) = \mathbf{g}\sum_{m=1}^{n} \nabla_m \nabla^m q^i.$$

So here we have full analogy of relation as in the case of the functional of smoothness suggested by Brackbill and Saltzman for domains and the method of Crowley-Winslow based on the Laplace equations.

2.6 Transformed Equations

The inverted system of the Euler-Lagrange equations has the following form:

$$\sum_{i,m=1}^{n} \mathbf{g}_{qr}^{im} \frac{\partial^2 s^k}{\partial q^i \partial q^m} = \det{}^{1/2}\mathbf{G}^{rs} \sum_{m=1}^{n} \frac{\partial}{\partial s^m}(\det{}^{1/2}\mathbf{G}^{rs}\mathbf{g}_{sr}^{mk}).$$

This is an elliptic quasi-linear system and its right-hand side does not depend on the transformation $s(q)$, which is found by the solution of the system. The control of adaptation is provided by the coefficients $\mathbf{g}_{qr}^{ir}$ and the right-hand expression of the system.

2.7 Examples of adaptive grids

To find the values of the function $s(q)$ the system of the Euler-Lagrange equations was solved in the domain Q^n. The boundary nodes were obtained by adaptation along the arc of the curve. The derivatives of the equations were approximated by the central differences and the right hand side of the equations was considered on the $(n-1)$th layer. Difference equations were solved by the SOR iterative method. As an initial guess an algebraic grid was taken which was constructed by the method of interpolation of boundary nodes. Figures 4 (a, b) show adaptive grids in domains. Figure 5 shows a grid on the cross-section plane obtained by calculations of a non-viscous gas flow around a cone in which the pressure function $p(x)$ was taken to form the monitor surface. Figures 6 (a,b) demonstrate the adaptive grids on the saddle surface. The adaptive grid on the sides of a curvilinear three-dimensional domain is shown on Figure 7. The numerical implementation of the method was carried out by Petrenko, Liseikin (1994) and Kupin, Liseikin (1994).

REFERENCES

Atlas, I. and Stephenson, J. W. (1991) A two-dimensional adaptive mesh generation method. *Journal of Computational Physics*, **94**, 201–224.

Aubin, J.-P. (1972) Approximation of elliptic boundary-value problems: Pure and Applied Mathematics, in A Series of Texts and Monographs, V, XXVI, (ed. R. Courant, L. Bers, J.J.Stoker).

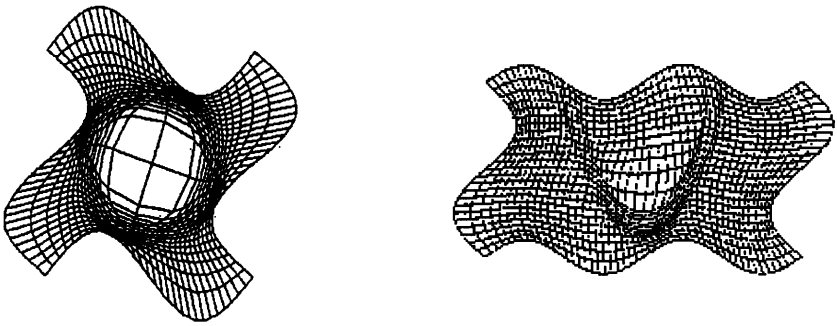

Figure 4 Adaptive grids in domains. Left is (a) and right is (b).

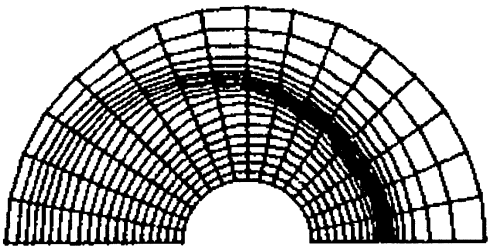

Figure 5 A grid on the cross-section plane obtained by calculations of a non-viscous gas flow around a cone in which the pressure function $p(x)$ was taken to form the monitor surface.

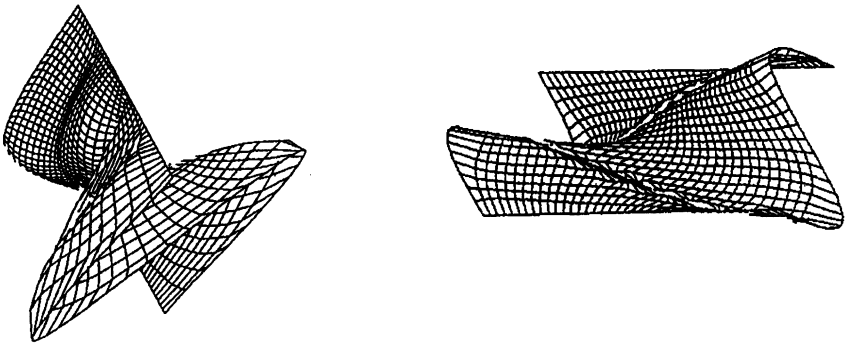

Figure 6 The adaptive grids on the saddle surface. Left is (a), right is (b).

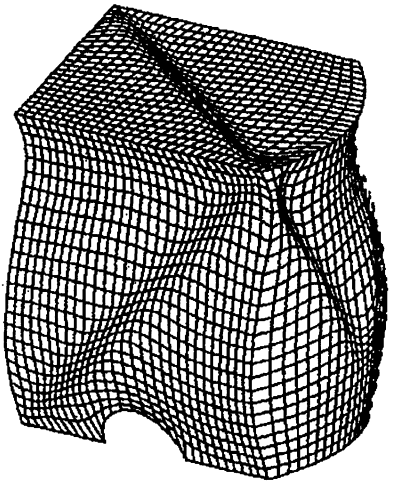

Figure 7 The adaptive grid on the sides of a curvilinear three-dimensional domain.

Ciarlet, P. (1978) The finite element method for elliptic problems. *Studies in Mathematics and Its Applications.* **4**, North-Holland Publishing Company, Amsterdam, New York, Oxford.

Gardner, M. (1988) Time travel and other mathematical bewilderment's, W.H.Freeman and Company, New York.

Kupin, E.P. and Liseikin, V.D. (1994) Method of projection for generation of multidimensional adaptive grids. *Computational Technologies*, **3**, 8, 189–198, (in Russian).

Lebedev, V. I., Agoshkov, V. I. (1983) Poincare-Steklov Operators and their Applications in to Analysis. OVM AN SSSR, Moscow, (in Russian).

Liseikin, V. D. (1991) The Construction of Regular Grids on n-Dimensional Surfaces. *Computer Mathematics and Mathematical Physics*, **31**, 11, 47–57.

Liseikin, V. D. (1993) On some interpretations of smoothness functional used in constructing regular and adaptive grids. *Russian Journal of Numerical Analysis and Mathematical Modelling*, **8**, 6, 507–518.

Liseikin, V. D. (1996a) Adaptive Grid Generation on the Basis of Smoothness Functional, in *Proceedings of V-th. International Conference on Numerical Grid Generation in Computational Field Simulations* (ed. by B.K. Soni, J.F.Thompson) MSU, **2**, 1131–1140.

Liseikin, V. D. (1996b) Survey of Adaptive Grid Generation Methods. *Computer Mathematics and Mathematical Physics*, **36**, 1, 3–41.

Liseikin, V. D. and Petrenko, V. E. (1994) On analytical and numerical investigations of the projection method for generation of adaptive grids. *Computational Technologies*, **3**, 9, 108–120, (in Russian).

Nepomnyatshikh, S. V. (1986) Domain Decomposition and the Schwartz Methods in subdomain for the approximated solution of elliptic boundary problems: Ph.D. Th. Computing Center of SD of USSR AS, Novosibirsk, (in Russian).

Oden, J. T., Demkowicz, L. (1991) h-p adaptive finite element methods in computational fluid dynamics. *Computer Methods in Applied Mechanics and Engineering*, **91**, 11–40.

Shokin, Yu. I., Sleptsov, A. G. (1995) Projective-mesh method with small angles in cells. *Russian Journal of Numerical Analysis and Mathematical Modelling*, **10** (5), 449–462.

Sleptsov, A. G. (1991a) On the convergence acceleration of linear iterations. *Russian Journal of Theoretical and Applied Mechanics*, **1**, 74–83.

Sleptsov, A. G. (1991b) On the convergence acceleration of linear iterations: II. *Russian Journal of Theoretical and Applied Mechanics*, **1**, 213–220.

Sleptsov, A. G. (1993) Grid-projection solution of elliptic problem for a irregular grid. *Russian Journal of Numerical Analysis and Mathematical Modelling*, **8** (6), 501–525.

Sleptsov, A. G., Shokin, Yu. I. (1995) Adaptive Projection-Grid Method for Elliptic Problems. *Reports of RAS*, **347** (2), (to be published in Russian).

Smelov, V. V. (1982) Iteration Process With Respect to Subdomains for the transport Problems in an odd P_{2N+1}-approximation. *Journal of Computational Mathematics and Mathematical Physics*, **22** (1), 151–162, (in Russian).

Strang, G., Fix, G. J. (1973) An analysis of the finite element method. Prentice-Hall, Ink, Englewood Cliffs, NJ.